Relativistic treatment of spin-currents and spin-transfer torque

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It is shown that a useful relativistic generalization of the conventional spin density $\vec{s}(\vec{r},t)$ for the case of moving electrons is the expectation value $(\vec{T}(\vec{r},t), T_4(\vec{r},t))$ of the four-component Bargmann-Wigner polarization operator $T_{\mu} = (\vec{T}, T_4)$ with respect to the four components of the wave function. An exact equation of motion for this quantity is derived, using the one-particle Dirac equation, and the relativistic analogues of the non-relativistic concepts of spin-currents and spin-transfer torques are identified. In the classical limit the time evolution of $(\vec{\tau}, \tau_4)$, the integral of $(\vec{T}(\vec{r},t), T_4(\vec{r},t))$ over the volume of a wave packet, is governed by the equation of motion first proposed by Bargmann, Michel and Telegdi generalized to the case of inhomogeneous systems. In the non-relativistic limit it is found that the spin-current has an intrinsic Hall contribution and to order $1/c^2$ a spin-orbit coupling related torque appears in the equation of motion for $\vec{s}(\vec{r},t)$. The relevance of these results to the theory of the intrinsic spin Hall effect and current-induced switching are briefly discussed.

PACS numbers: 71.70.Ej, 72.25.-b, 75.60.Jk, 85.75.-d

Central to the emerging technology of spin-based electronics, often referred to as spintronics, is the observation that electron transport can be influenced not only by coupling to the charge but also to the spin of the current carrying electrons. [1] A striking example of charge-current being effected by the magnetic state of the conductor is the giant magneto-resistance (GMR) phenomenon. Evidently, the complementary effects of charge-currents inducing changes in the magnetization of the conductors are also of interest. An example of these is the currentinduced switching first predicted by J. C. Slonczewski and independently by L. Berger. [2, 3] As is now well established, it is due to the spin-transfer torque that a spin-polarized current can exert on the magnetization of the structure through which it flows. [4] However, the details of how such torques come about have not been, as yet, fully explored. In particular, all discussions of the problem are currently based on non-relativistic quantum mechanics and hence neglect the spin-orbit coupling. The purpose of this letter is to present a fully relativistic theory of spin-currents and the above spin-transfer torque in order to provide a conceptual framework in which the spin and orbital degrees of freedoms can be treated on equal footing.

Another topic, to which such developments are relevant, is the spin Hall effect intensively studied in semi-conductor spintronics. [5, 6] It involves a spin-current flowing perpendicularly to a charge-current in a sample of finite width. Interestingly, it implies spin accumulation at the edges and the possibility of spin-injection into an adjacent sample without the presence of magnetic or exchange fields. Here, spin-orbit coupling is the central issue and a source of difficulty is the lack of a well-defined spin-current in a spin-orbit coupled system. [6] It is hoped that the polarization-current introduced in this letter will clarify this matter considerably.

A moving electron carries with it a spin and this moving spin amounts to a spin-current. Classically, it is given by the tensor product, $\overrightarrow{J}_{\rm cl} = \overrightarrow{s}_{\rm cl} \otimes \overrightarrow{v}$, of the velocity vector \overrightarrow{v} and a classical spin vector $\overrightarrow{s}_{\rm cl}$. Quantum mechanically, for an electron described by a two-component wave function $\phi = \begin{pmatrix} \phi_{\uparrow} \\ \phi_{\downarrow} \end{pmatrix}$, with spin components ϕ_{\uparrow} and ϕ_{\downarrow} , it is given by the tensor density

$$\overleftrightarrow{J}_{s} = \phi^{+} \left(\vec{\sigma} \otimes \vec{J} \right) \phi , \qquad (1)$$

where $\vec{J} = i\hbar \left(\overleftarrow{\nabla} - \overrightarrow{\nabla} \right) / (2m_{\rm e})$, the wave functions and therefore also the spin-current $\overrightarrow{J}_{\rm s}$ are evaluated at the space time point (\vec{r}, t) . The physical significance of $\overrightarrow{J}_{\rm s}$ becomes apparent if we study the time evolution of the spin density defined by $\vec{s} = \phi^+ \vec{\sigma} \phi$. From the time-dependent Schrödinger equation which includes a Zeeman term of the form $-\mu_{\rm B} \vec{\sigma} \cdot \vec{B}$ we find

$$\frac{d\vec{s}}{dt} + \nabla \cdot \stackrel{\longleftrightarrow}{J}_{s} = \frac{e}{m_{e}} \vec{s} \times \vec{B} . \tag{2}$$

Clearly, $\nabla \cdot \overrightarrow{J}_{\mathrm{s}}$ may be regarded as a torque which, in addition to the more familiar microscopic Landau-Lifshitz torque $\overrightarrow{s} \times \overrightarrow{B}$, causes the spin density \overrightarrow{s} at the point \overrightarrow{r} to evolve in time. As explained, at length, in the insightful review of Stiles and Miltat this spin-transfer torque depends linearly on the charge-current and plays a central role in current-induced switching. [4]

Note that for $\vec{B}=0$ Eq. (2) is a continuity equation for the spin density \vec{s} and as such it follows via the Noether theorem from the fact that \vec{s} is a conserved quantity. The difficulty of generalizing the continuity equation to spin-orbit coupled systems, such as described by the Dirac equation or by various model Hamiltonians, e.g., like those used in semiconductor spintronics, [6, 7] arises from

the circumstance that in these cases the spin operator no longer commutes with the Hamiltonian and hence the conventional spin density is not conserved as the time evolves. In what follows this dilemma is resolved by the choice of a convenient, covariant description of the spin-polarization, as an alternative to that afforded by the usual spin operators in non-relativistic quantum mechanics. In the following, for the sake of simplicity only the case of non-interacting positive energy Dirac electrons will be considered.

For electrons described by the Dirac equation in the standard representation it is common to refer to

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \tag{3}$$

as the 4×4 Pauli spin operator. However, it corresponds to the spin of an electron only in its rest frame and hence its use is not convenient in the case of many moving electrons. Moreover, as mentioned above, it does not commute even with the field-free Dirac Hamiltonian $\mathcal{H}_{\rm D} = c\vec{\alpha} \cdot \vec{p} + \beta m_{\rm e}c^2$ and hence the corresponding density is not that of a conserved quantity. A more suitable approach for describing the spin-polarization of moving electrons is to use the four-component polarization operator $T_{\mu} \equiv (\vec{T}, T_4)$ introduced by Bargmann and Wigner. [8] The salient features of this approach and its relations to other, alternatives, are fully discussed in a comprehensive review article by Fradkin and Good. [9] Here they will be merely referred to as the need arises.

For the case of one electron, in the presence of an electromagnetic field described by the vector potential $\vec{A} = \vec{A}(\vec{r},t)$ and a scalar potential $V = V(\vec{r},t)$, the four-component polarization operator is defined by

$$\begin{cases}
\vec{T} = \beta \vec{\Sigma} - i\Sigma_4 \frac{\vec{\Pi}}{m_e c} \\
T_4 = i \vec{\Sigma} \cdot \frac{\vec{\Pi}}{m_e c}
\end{cases}$$
(4)

where the canonical momentum operator takes its usual form: $\vec{\Pi} = (\vec{p} - e\vec{A})I_4$, with I_4 being the 4×4 unit matrix, $\vec{\Sigma}$ is the spin operator defined in Eq. (3). For future reference note that $\vec{\Sigma}$ is part of the four-component operator $\Sigma_{\mu} \equiv (\vec{\Sigma}, \Sigma_4)$ whose 4th component is defined as $\Sigma_4 = -i \gamma_5$, see e.g. Ref. 10. It is also of interest to note that both T_{μ} and Σ_{μ} are covariant axial four-vectors.

From the point of view of our present concern the most important property of T_{μ} is that commutes with the field-free Dirac Hamiltonian. Thus, as will be shown below, the corresponding vector density satisfies a continuity equation. To see the connection between the non-relativistic spin operator $\vec{\sigma}$ and \vec{T} it is useful to note that the latter is related to the magnetization of an electron in its rest frame by a Lorentz boost.

To derive a relativistic analogue of Eq. (2) one has to calculate the first derivative with respect to the time of the polarization densities $\vec{\mathcal{T}} = \vec{\mathcal{T}}(\vec{r},t)$ and $\mathcal{T}_4 = \mathcal{T}_4(\vec{r},t)$ defined by

$$\vec{T} = \psi^+ \vec{T} \psi$$
 and $T_4 = \psi^+ T_4 \psi$,

where $\psi^+ = \psi^+(\vec{r},t)$ is the adjoint (conjugate transpose) of the four-component solution $\psi = \psi(\vec{r},t)$ of the time-dependent Dirac equation corresponding to the Hamiltonian $\mathcal{H}_{\rm D} = \mathcal{H}_{\rm D}(\vec{r},t) = c\vec{\alpha} \cdot \vec{\Pi} + \beta m_{\rm e}c^2 + eVI_4$. By using the chain rule for all four components $\mu = 1, \ldots, 4$ in Eq. (4),

$$\frac{d\vec{\mathcal{T}}_{\mu}}{dt} = \frac{\partial \psi^{+}}{\partial t} T_{\mu} \psi + \psi^{+} \frac{\partial T_{\mu}}{\partial t} \psi + \psi^{+} T_{\mu} \frac{\partial \psi}{\partial t} ,$$

and the relations

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \mathcal{H}_{\mathrm{D}} \psi , \qquad \frac{\partial \psi^{+}}{\partial t} = -\frac{1}{i\hbar} \psi^{+} \mathcal{H}_{\mathrm{D}}^{+}$$

$$\frac{\partial \vec{T}}{\partial t} = \gamma_5 \frac{e}{m_e c} \frac{\partial \vec{A}}{\partial t} , \qquad \frac{\partial T_4}{\partial t} = -\frac{ie}{m_e c} \vec{\Sigma} \cdot \frac{\partial \vec{A}}{\partial t} ,$$

after some lengthy but straightforward algebra one arrives at

$$\frac{d\vec{\mathcal{T}}}{dt} + \nabla \cdot \overleftrightarrow{\mathcal{J}}' + \nabla \mathcal{J}'' = \frac{e}{m_{\rm e}} \vec{\mathcal{S}} \times \vec{B} - \frac{ie}{m_{\rm e}c} \vec{E} \,\mathcal{S}_4 \;, \quad (5)$$

and

$$\frac{d\mathcal{T}_4}{dt} + \nabla \cdot \left(\vec{\mathcal{J}_4}' - \vec{\mathcal{J}_4}''\right) = \frac{ie}{m_e c} \vec{\mathcal{S}} \cdot \vec{E} , \qquad (6)$$

where $\vec{B} = \vec{B}(\vec{r}, t)$ is the magnetic induction vector and $\vec{E} = \vec{E}(\vec{r}, t)$ the electric field intensity. In Eqs. (5) and (6), the four-component density $S_{\mu} \equiv (\vec{S}, S_4)$ is given by

$$\vec{\mathcal{S}} = \psi^{+} \vec{\Sigma} \, \psi, \qquad \mathcal{S}_4 = \psi^{+} \Sigma_4 \psi$$

and the polarization-current density tensors are defined as

$$\overrightarrow{\mathcal{J}}' = c \psi^{+} \left(\overrightarrow{T} \otimes \overrightarrow{\alpha} \right) \psi \qquad \overrightarrow{\mathcal{J}}_{4}' = c \psi^{+} \left(T_{4} \overrightarrow{\alpha} \right) \psi$$

$$\mathcal{J}'' = \psi^{+} \left(2c \beta \gamma_{5} \right) \psi \qquad \overrightarrow{\mathcal{J}}_{4}'' = \psi^{+} \left(2 \frac{\overrightarrow{\pi}}{m_{e}} \times \overrightarrow{\alpha} \right) \psi$$
(7)

such that

$$\nabla \cdot \overleftrightarrow{\mathcal{J}}' = \sum_{j=x,y,z} \partial_j \left[\psi^+ \left(\vec{T} \alpha_j \right) \psi \right] .$$

Although the above relations bear some resemblance to Eq. (2) the problem of generalizing it to relativistic quantum mechanics is not yet completed because Eqs. (5) and (6) are not a closed set of equations for the polarization

density in terms of corresponding currents. To proceed further one must derive the equation of motion for the four-component auxiliary density S_{μ} . Following the same route as in the case of $\mathcal{T}_{\mu} \equiv (\vec{\mathcal{T}}, \mathcal{T}_4)$ one straightforwardly finds that

$$\frac{d\vec{S}}{dt} - ic \nabla S_4 = \frac{m_e c}{\hbar} \vec{\mathcal{J}}_4^{"} + i \nabla \times \vec{\mathcal{J}}$$
 (8)

and

$$i\frac{dS_4}{dt} - c\nabla \cdot \vec{S} = i\frac{m_e c}{\hbar} \mathcal{J}'', \qquad (9)$$

with $\vec{\mathcal{J}} = c \psi^+ \vec{\alpha} \psi$ being the relativistic probability current density. Remarkably, some of the same currents which appear in the equations for \mathcal{T}_{μ} determine \mathcal{S}_{μ} and hence for a given set of currents in Eq. (7), Eqs. (5), (6), (8) and (9) can be solved for \mathcal{T}_{μ} and \mathcal{S}_{μ} .

The relations in Eqs. (5) - (9) are the central result of this letter. Namely, the comparison of Eqs. (2) and (5), without electromagnetic fields, uniquely identifies the polarization-current density as $\overrightarrow{\mathcal{J}}' + \mathcal{J}'' \mathbf{I}_3$ and its divergence as the relativistic generalization of the conventional spin-current density and spin-transfer torque, respectively. Indeed, in the case of a vanishing electromagnetic field Eq. (5) reduces to a continuity equation for the polarization density in the same manner as Eq. (2) is a continuity equation for the magnetization density.

To shed light on the physical content of these results they will now be examined in two separate limits. First the classical, $\hbar \to 0$, then the non-relativistic, $c^{-2} \to 0$ limit will be studied.

The aim of the classical limit is to find a dynamical description of the polarization of an electron whose orbital motion is classically given by the position vector $\vec{r}_{\rm cl}(t)$ as prescribed by a relativistic classical mechanical equation of motion. This is the case of interest in Ref. 9 and phenomenologically is treated in Ref. 11. In short one assumes that $\psi(\vec{r},t)$ describes a wave packet centered at the position vector $\vec{r}_{cl}(t)$ and moving with a velocity $\vec{v}_{\rm cl}$. The size of the wave packet is to be taken to be large compared with the Compton wave length \hbar / mc but very much smaller then the scale on which the external electromagnetic field vary. Moreover, it contains momentum components only near $m_{\rm e}\vec{v}_{\rm cl}$. In the lights of these assumptions it is natural to define a four-vector $\tau_{\mu} = (\vec{\tau}, \tau_4)$ as the integral of the density \mathcal{T}_{μ} over the variable \vec{r} within a volume Ω as

$$\vec{\tau} \equiv \vec{\tau}(t) = \int_{\Omega} d^3r \, \vec{T}(\vec{r}, t) , \quad \tau_4 \equiv \tau_4(t) = \int_{\Omega} d^3r \, T_4(\vec{r}, t)$$

and derive an equation of motion for $\tau_{\mu}(t)$ from those for \mathcal{T}_{μ} as given in Eqs. (5) and (6). Evidently, the property $\tau_{\mu}(t)$ is to be associated with a classical particle described by $\vec{r}_{\rm cl}(t)$ and $\vec{v}(t)$. Following the procedure of Ref. 9 we

ind

$$\frac{d\vec{\tau}}{dt} + \int_{\Omega} d^3r \, \nabla \cdot \stackrel{\longleftrightarrow}{\mathcal{J}}'(\vec{r}, t) \bigg|_{\text{cl}} = \bar{\gamma}^{-1} \, \vec{\tau} \times \vec{B}(\vec{r}_{\text{cl}}, t) \qquad (10)$$

$$- i \frac{e}{m_e c} \bar{\gamma}^{-1} \, \tau_4 \vec{E}(\vec{r}_{\text{cl}}, t) ,$$

where $\bar{\gamma}$ is the Lorentz factor $\left(1-v^2/c^2\right)^{-1/2}$ and , as indicated, the external fields are evaluated at the current position $\vec{r}_{\rm cl}(t)$ of the particle. Noting the result $\langle \mathcal{S}_{\mu} \rangle \simeq \bar{\gamma}^{-1} \tau_{\mu}$ of Ref. 9, where $\langle \mathcal{S}_{\mu} \rangle$ denotes the classical limit of the density \mathcal{S}_{μ} integrated over Ω , the form of the right-hand side of the above relation readily follows from Eq. (5). The term involving \mathcal{J}'' was also shown to be zero by following the procedure of Ref. 9.

Before commenting on its most interesting feature, namely the torque on the left-hand side, it is reassuring to note that without it Eq. (10) is exactly that of Bargmann, Michel and Telegdi (BMT) [12] discussed at length by Landau. [11] The extra factor of $\bar{\gamma}$ is due to the fact that the derivative on the left-hand side is with respect to the global time t and not the proper time in the rest frame of the electron as in Ref. 11. To clarify the physical content of the BMT equation, Landau introduces a classical spin polarization vector in the rest frame, here denoted by $\vec{s}(t)$, and demands that when it is Lorentz boosted into the global frame, $\vec{s}(t)$ would be equal to $\vec{\tau}(t)$ in this letter. This allows him to convert the equation for $\vec{\tau}(t)$ to one describing $\vec{s}(t)$. In the interest of brevity his result is recalled here only to order c^{-2} :

$$\frac{d\vec{s}}{dt} \simeq \frac{e}{m_e c} \, \vec{s} \times \vec{B} + \frac{e}{2m_e c} \, \vec{s} \times \left(\vec{E} \times \frac{\vec{v}}{c} \right) \; . \label{eq:delta}$$

Clearly, the second term on the right-hand side is a torque – due to an effective magnetic induction vector $\vec{E} \times \vec{v}/c$ – a moving electron experiences in an electric field \vec{E} . In other words it is the simplest manifestation of spin-orbit coupling. For example, a Rashba Hamiltonian analogue of this term is the main mechanism of the intrinsic spin Hall effect in the work of Sinova et al. [13]

The novel and the most interesting feature of Eq. (10) is the torque on the left-hand side. For a uniform $\overrightarrow{\mathcal{J}}'$, e.g., in a bulk material, $\nabla \cdot \overrightarrow{\mathcal{J}}'$ is zero. But when the effective classical particle crosses an interface or a domain wall with spin-dependent properties, the volume integral can be converted into an integral over a closed surface. If this surface includes the interface, whose differential oriented surface is $d\vec{A}$, then the torque is $(\overrightarrow{\mathcal{J}}'^+ - \overrightarrow{\mathcal{J}}'^-) \cdot d\vec{A}$, where \pm refers to the opposite sites of the interface. Thus, just as in the non-relativistic case, see Ref. 5, this torque is due to an excess in the spin-current flowing in and out of the surface region causing a polarization accumulation. This then supports in very explicit terms, the identification of $\overrightarrow{\mathcal{J}}' + \mathcal{J}'' \mathbf{I}_3$ as the fully relativistic generalization of the non-relativistic definition

of spin-current. Notably, in the classical limit one might approximate $\overleftrightarrow{\mathcal{J}}' \simeq \vec{\tau} \otimes \vec{u}$, where \vec{u} is the relativistic velocity vector $\bar{\gamma}\vec{v}$ and $\vec{\tau}$ is described by the BMT equation (10). This is a rather satisfactory result given the form of the non-relativistic classical formula $\overleftrightarrow{\mathcal{J}}' \simeq \vec{s} \otimes \vec{v}$ quoted at the beginning of this letter.

Finally, in what follows we examine the lowest order corrections to the non-relativistic theory. Working to the order 1/c, after considerable algebra we find that the equations for $\vec{\mathcal{T}}$ and $\vec{\mathcal{S}}$ satisfy one and the same equation of motion, and the polarization-current is given by

Evidently, the first two terms in Eq. (11) are the generalization of the conventional \overrightarrow{J}_s in Eq. (1) to the case of a non-vanishing vector potential. The third term $\delta \overrightarrow{\mathcal{J}}^{(1)}$ is a consequence of the internal contribution to the probability current density due to the moving dipole moment $\delta \overrightarrow{J}_{int} = \hbar \nabla \times (\phi^+ \overrightarrow{\sigma} \phi) / (2m_e)$, [11] and its form readily follows from the anzatz $\delta \overrightarrow{\mathcal{J}}^{(1)} = \phi^+ (\overrightarrow{\sigma} \otimes \delta \widehat{\overrightarrow{J}}_{int}) \phi$. [14] Moreover, just as $\delta \overrightarrow{J}_{int}$ does not contribute to the divergence in the continuity equation for the probability density, $\nabla \cdot \delta \overrightarrow{\mathcal{J}}^{(1)}$ is identically zero and gives rise to no torque.

To the order of $1/c^2$ there are many more contributions. These will be discussed in a separate publication. Here only one term $\delta \overrightarrow{\mathcal{J}}_{\mathrm{SOC}}^{(2)}$, which is clearly to be associated with the spin-orbit coupling, is highlighted:

$$\delta \overrightarrow{\mathcal{J}}_{SOC}^{(2)} = \frac{ie\hbar}{2m_{e}^{2}c^{2}} \vec{E} \cdot \left(\tilde{\phi}^{+}\vec{\sigma}\tilde{\phi}\right) \mathbf{I}_{3}$$

$$+ \frac{e\hbar}{2m_{e}^{2}c^{2}} \begin{pmatrix} 0 & +E_{z} & -E_{y} \\ -E_{z} & 0 & +E_{x} \\ +E_{y} & -E_{x} & 0 \end{pmatrix} \left(\tilde{\phi}^{+}\tilde{\phi}\right) ,$$

$$(12)$$

where $\tilde{\phi}$ is ϕ renormalized as in Ref. 11.

Remarkably, the off-diagonal terms have the form required by the spin Hall effect. [6] It means that for example an electric field, and presumably a charge-current, along the z axis, a spin polarization along the x axis implies a polarization-current in the y direction. Interestingly, this term is the only contribution obtained, if one uses, in a simple minded derivation, the anomalous velocity, [15] $\vec{v}_a = -e\hbar (\vec{\sigma} \times \vec{E})/(4m_e^2c^2)$, and the non-relativistic definition of the spin-current density $\tilde{\phi}^+[\vec{\sigma}\otimes\vec{v}+(\vec{v}\otimes\vec{\sigma})^T]\tilde{\phi}$. [6, 14] Thus the first term in Eq. (12) is a nontrivial consequence of our more general, fully relativistic treatment of the polarization. Clearly, it implies that for a charge current along the electric field there will be a helicity dependent contribution to the spin-current.

Whilst the above reference to the spin Hall effect can not be taken as an explanation for the observed spin Hall currents due to the smallness of the vacuum coupling constant $\lambda_{\rm SOC} = e\hbar / (2m_{\rm e}^2c^2)$, see Ref. 6, the presence of a relevant term in Eq. (12) suggests that an intrinsic spin Hall effect is a generic feature of spin-orbit coupled systems and therefore of the relativistic quantum mechanics.

In conclusion it should be stressed that the above discussion was confined to a one-electron theory based on a one-electron Dirac equation. Nevertheless, the results establish the line of reasoning a relativistic generalization of the corresponding many-particle theory has to take. In particular it will lead to a relativistic version of the semi-classical transport theory for the current-induced switching dynamics, [4] or for that of the spin Hall effect. [16] It will also facilitate the corresponding generalization of the time-dependent density functional theory of Capelle et al., [17] and will readily provide a framework for first-principles calculation using fully relativistic methods such as the screened RKKR. [18] Interestingly, it will also enter the relativistic Fermi liquid theory of Baym and Chin. [19]

Financial support by the Vienna Science and Technology Fund (WWTF), the Wolfgang-Pauli Institut (WPI) and the Vienna Institute of Technology (TU Vienna) is gratefully acknowledged.

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